Hartree-Fock-Bogoliubov theory without quasiparticle vacua

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Hartree-Fock-Bogoliubov (HFB) theory is generalized by eliminating the restriction to quasiparticle vacuum states. However, the fundamental HFB transformation to quasiparticles is retained. The theory is formulated in terms of the quasiparticle density matrix R, but, in contrast to conventional HFB, there is no restriction to vacuum densities $R^2 = R$.

I. INTRODUCTION

Recently, Hartree-Fock (HF) theory was generalized to apply to nondeterminantal densities, while retaining the essential HF approximation of one-body dynamics.[1,2] This new generalization exploits the fundamental role played by the group $U(n)$ of unitary transformations in the n-dimensional single-particle space, both in characterizing the restricted space of HF densities and determining the dynamical law on that space.

For example, in ordinary HF, if ρ is a fixed, but arbitrary, determinantal density ($\rho^2 = \rho$), then every other determinantal density is in the unitary orbit of densities,

$$O_\rho = \{g\rho g^{-1} | g \in \mathrm{U}(n)\}. \tag{1}$$

This orbit may be regarded as a surface in the space of all densities and a time-dependent Hartree-Fock (TDHF) solution is a curve lying in this surface. At each point on the surface, the HF Hamiltonian is an element of the Lie algebra of $U(n)$, i.e., a one-body operator, and has the geometrical interpretation of a tangent vector to the surface at the point. Furthermore, the Lie algebra structure gives O_ρ the geometry of a symplectic manifold or phase space, and the TDHF equations are identical to classical Hamiltonian equations of motion.

In the extension of HF defined in Ref. 2, the space of states is again an orbit O_ρ, but ρ is not required to be determinantal. Thus, all possible orbit surfaces in the space of densities are admissible. The generalized HF Hamiltonian also has the geometrical interpretation of a vector field tangent to the surface O_ρ and is, at each point of O_ρ, a one-body operator. Moreover, the phase-space structure persists for the general orbits, and dynamics is determined by the classical Hamiltonian dynamical law. Since the surfaces O_ρ are co-adjoint orbits of $U(n)$, the interrelated group and symplectic structures on it are no accident, but rather reflect a general theorem applicable to co-adjoint orbits of Lie groups.[3-5]

In this paper, Hartree-Fock-Bogoliubov (HFB) theory is generalized using analogous ideas. The relevant group for HFB is $\mathrm{O}(2n)$, the orthogonal group in $2n$ dimensions.[6,7] Its Lie algebra properly contains the one-body operators spanning $u(n)$, the HF algebra. In addition, the $\mathrm{O}(2n)$ algebra includes the fermion pair creation and pair annihilation operators. Thus, the HFB Hamiltonian is an element of the orthogonal Lie algebra. The proof of these facts is reviewed in the appendix; reviews of HFB have been given by Goodman[8] and Mang.[9]

In place of the density ρ, one now considers the generalized HFB density R and its co-adjoint orbit,

$$O_R = \{gRg^{-1} | g \in \mathrm{O}(2n)\}. \tag{2}$$

In conventional HFB, the density is idempotent, $R^2 = R$, since it corresponds to a quasiparticle vacuum wave function. Moreover, every density in the orbit O_R is idempotent, $(gRg^{-1})^2 = gRg^{-1}$, and, conversely, every quasiparticle vacuum defines a density in the orbit O_R with R a fixed idempotent, but otherwise arbitrary, generalized density. Indeed, the co-adjoint action $R \to gRg^{-1}$ refers to the transformation of the density induced by the quasiparticle transformation associated with $g \in \mathrm{O}(2n)$. But, every quasiparticle vacuum may be obtained from a fixed quasiparticle vacuum wave function by an orthogonal quasiparticle basis transformation.

It is useful to adopt a geometrical viewpoint with the density matrices. Consider O_R, the orbit of quasiparticle vacuum densities, as a surface contained within the space of all possible generalized density matrices. The exact Hamiltonian $\hat{H}$ may be regarded as a vector field which is directed, in general, off the surface. On the other hand, the HFB Hamiltonian H_{HFB} is a vector field which is everywhere tangent to the orbit surface. Subsequently, it will also be shown that this surface is a phase space (symplectic manifold) and that H_{HFB} is constructed from $\hat{H}$ by projection relative to the nondegenerate symplectic form. An HFB

solution is defined as a point on the surface for which the HFB Hamiltonian is the zero tangent vector.

Physically, constraint to an $O(2n)$ orbit surface means, by definition, a restriction to quasiparticle dynamics. This is because the generators of the orthogonal group are precisely the generators of quasiparticle transformations. The crucial point is that this physical interpretation applies not only to the orbit of idempotent quasiparticle vacuum densities, but also to every $O(2n)$ orbit surface. Hence, we are led to consider the continuum of all possible orbits O_R each of which defines constrained quasiparticle dynamics. Only one of these surfaces in the space of all generalized densities, the orbit O_R with $R^2=R$, demands that the densities correspond to quasiparticle vacua. The general orbits provide the framework for the generalization of conventional HFB investigated in this article.

The plan of this paper is to define the phase space structure on the generalized orbits in Sec. II. In Sec. III, this symplectic geometry provides an explicit construction for the generalized HFB Hamiltonian from the exact Hamiltonian. A discussion of this generalization closes the article.

II. CO-ADJOINT ORBITS

The Lie algebra relevant to HFB consists of the Hermitian bilinear projects of fermion creation and annihilation operators. Because of the symmetrical way in which the creation and annihilation operators enter into HFB, it is convenient to define the $2n$ operators $d_\alpha^\dagger$, $1\leq\alpha\leq 2n$, where for the first n operators $d_\alpha^\dagger=a_\alpha^\dagger$, the creation operator for the single-particle state α, and for the last n operators $d_\alpha^\dagger=a_\alpha$, the annihilation operator for the state α. We assume, for simplicity, that the single-particle space has finite dimension n.

An element $\hat{Z}$ of the orthogonal algebra $o(2n)$ is given by

$$\hat{Z}=\tfrac{1}{2}\sum_{\alpha\beta}Z_{\alpha\beta}d_\alpha^\dagger d_\beta, \tag{3}$$

where Z is an Hermitian $2n\times 2n$ matrix of the form

$$Z=\begin{pmatrix} X & Y \\ Y^\dagger & -X^t \end{pmatrix}, \tag{4}$$

with X Hermitian and Y antisymmetric.

Fundamentally, a generalized HFB density R is an element of the dual of the Lie algebra $o(2n)$, i.e., a real-valued function of $Z\in o(2n)$. To be explicit, let R denote the HFB density matrix corresponding to the many-particle state Φ,

$$R_{\alpha\beta}=\langle\Phi\,|\,d_\beta^\dagger d_\alpha\Phi\rangle. \tag{5}$$

Thus, in terms of the HF density matrix ρ and the pairing tensor t,

$$R=\begin{pmatrix} \rho & t \\ t^\dagger & 1-\rho^t \end{pmatrix}, \tag{6}$$

where

$$\begin{aligned}\rho_{\alpha\beta}&=\langle\Phi\,|\,a_\beta^\dagger a_\alpha\Phi\rangle,\\ t_{\alpha\beta}&=\langle\Phi\,|\,a_\beta a_\alpha\Phi\rangle.\end{aligned} \tag{7}$$

Then, R defines a linear real-valued function of Z,

$$R(Z)=\langle\Phi\,|\,\hat{Z}\Phi\rangle=\tfrac{1}{2}\mathrm{tr}(RZ). \tag{8}$$

The quasiparticle transformation of the many-body states $\Phi\to\hat{g}\Phi$ for $g\in O(2n)$ induces the so-called adjoint action on the Lie algebra,

$$\hat{Z}\to\hat{g}\hat{Z}\hat{g}^{-1}=\sum_{\alpha\beta}\mathrm{Ad}_g(Z)_{\alpha\beta}d_\alpha^\dagger d_\beta, \tag{9}$$

since

$$\begin{aligned}d_\alpha^\dagger(g)&=\hat{g}d_\alpha^\dagger\hat{g}^{-1}=\sum_{\alpha'}d_{\alpha'}^\dagger g_{\alpha'\alpha},\\ d_\alpha(g)&=\hat{g}d_\alpha\hat{g}^{-1}=\sum_{\alpha'}g^{-1}_{\alpha\alpha'}d_{\alpha'},\end{aligned} \tag{10}$$

and the adjoint action on $o(2n)$ is defined by

$$\mathrm{Ad}_g(Z)=gZg^{-1} \tag{11}$$

for all $Z\in o(2n)$ and $g\in O(2n)$. As reviewed in the Appendix, the quasiparticle transformations g form a subgroup of the $2n\times 2n$ unitary matrices isomorphic to the orthogonal group $O(2n)$.

The adjoint action induces the co-adjoint action Ad_g^* on the generalized densities,

$$\mathrm{Ad}_g^*(R)=gRg^{-1}. \tag{12}$$

This co-adjoint action is compatible with the action of $O(2n)$ on the many-particle states,

$$\mathrm{Ad}_g^*(R)(Z)=\langle\hat{g}\Phi|\,\hat{Z}\hat{g}\Phi\rangle. \tag{13}$$

Note that in order to use conventional physics notation, R and Z are Hermitian, whereas in mathematical literature the dual elements R and the Lie algebra elements Z are skew Hermitian. However, this discrepancy is purely notational and has no deep significance.

In order to define symplectic geometry on the orbit surfaces, it is first necessary to characterize O_R in a manageable way. Note that if Φ is a state with fixed particle number A, then the pairing tensor is zero. Moreover, by a unitary transformation of the single-particle basis, the HF density ρ may be diagonalized. Therefore, the physically relevant orbits are enumerated by the set

of O_R as R ranges over the diagonal generalized densities,

$$R=\begin{pmatrix}\rho & 0\\ 0 & 1-\rho\end{pmatrix},\quad \rho=\mathrm{diag}(\nu_1,\ \nu_2,\ldots,\nu_n). \tag{14}$$

The quasiparticle vacua form the orbit with $\rho=\mathrm{diag}(1,\ 1,\ldots,1,\ 0,\ldots,0)$. The generic orbits correspond to densities with distinct occupancies, $\nu_\alpha\neq\nu_\beta$ for $\alpha\neq\beta$, and $\nu_\alpha+\nu_\beta\neq 1$, $\sum\nu_\alpha=A$.

An orbit surface O_R is in one-to-one correspondence with the coset space of $O(2n)$ modulo the isotropy subgroup at R,

$$H_R=\{h\in O(2n)\,|\,hRh^{-1}=R\}. \tag{15}$$

The identification of the coset space with the orbit surface is given by

$$O(2n)/H_R\to O_R,$$
$$gH_R\to gRg^{-1}. \tag{16}$$

This mapping is clearly onto the orbit. It is also one-to-one, since if g_1 and g_2 define the same density, $g_1Rg_1^{-1}=g_2Rg_2^{-1}$, then $g_2^{-1}g_1\in H_R$ and, hence by definition, g_1 and g_2 are in the same coset, $g_1H_R=g_2H_R$.

Geometry on each orbit is determined by the Lie algebra $o(2n)$. Fix a diagonal generalized density R and its orbit O_R. Every Lie algebra element Z in $o(2n)$ defines a curve $\gamma_z(t)$ through the point R and lying entirely in the surface O_R, $\gamma_z(t)=\exp(itZ)R\exp(-itZ)$. The tangent vector to the curve γ_z at R may be identified with Z itself.

Note, however, that the elements of the isotropy subalgebra h_R define zero tangent vectors. This follows because if $Z\in h_R$, then $\exp(itZ)$ is in the isotropy subgroup H_R and, hence, $\gamma_z(t)=R$, a fixed point. Therefore, nonzero tangent vectors must correspond to a complementary subspace to h_R in $o(2n)$. Although no unique choice for this complementary subspace presents itself, a convenient selection is given by the subspace $h_R^\perp$ orthogonal to h_R relative to the Killing form κ. The tangent space at R is given by

$$h_R^\perp=\{Z\in o(2n)\,|\,\kappa(Z,Z')\equiv\mathrm{tr}(ZZ')=0,\ \text{for all } Z'\in h_R\}. \tag{17}$$

Consider next the description of the tangent space at an arbitrary point gRg^{-1} on O_R. Once again, every $Z\in o(2n)$ defines a curve through that point, viz. $\exp(itZ)gRg^{-1}\exp(-itZ)$. But, zero tangent vectors are given now by $Z\in gh_Rg^{-1}$, i.e., $Z=gZ'g^{-1}$, $Z'\in h_R$. Hence, the tangent space at gRg^{-1} is identified with the orthogonal complement $(gh_Rg^{-1})^\perp=gh_R^\perp g^{-1}=\mathrm{Ad}_g(h_R^\perp)$.

In order to complete the geometrical picture of O_R, it only remains to define the symplectic structure. The symplectic form ω at the point gRg^{-1} on the orbit O_R is an antisymmetric form defined on pairs of tangent vectors Z_1, Z_2 at gRg^{-1} by

$$\omega_{gRg^{-1}}(Z_1,Z_2)\equiv\frac{-i}{2}\mathrm{tr}(gRg^{-1}[Z_1,Z_2]). \tag{18}$$

In the special case of the orbit of quasiparticle vacua, this definition agrees with that defined for surfaces of wave functions in Ref. 1,

$$\omega_{gRg^{-1}}(Z_1,Z_2)=-i\langle\hat g\Phi|\,[\hat Z_1,\hat Z_2]\,\hat g\,\Phi\rangle\,. \tag{19}$$

The orthogonal group is a group of canonical transformations of O_R because the symplectic structure is preserved,

$$\omega_R(Z_1,Z_2)=\omega_{gRg^{-1}}(\mathrm{Ad}_g(Z_1),\mathrm{Ad}_g(Z_2))\,, \tag{20}$$

for pairs of tangent vectors Z_1, Z_2 at R. A key property of ω is that it is nondegenerate at every point, i.e., if $\omega_{gRg^{-1}}(Z,Z')=0$ for every tangent vector Z', then Z is the zero tangent vector.

The existence of the nondegenerate form ω implies that every orbit O_R is even dimensional and can be coordinatized by canonical coordinates q_i, p_i, if so desired. Moreover, the specification of ω is equivalent to a Poisson bracket operation on O_R[3].

Consider the concrete application of these general ideas to the various orbits. A basis for the Lie algebra $o(2n)$ is given by

$$\begin{aligned}
Q_{\alpha\beta}&=2^{-1/2}[(E_{\alpha\beta}+E_{\beta\alpha})-(E_{\alpha+n,\beta+n}+E_{\beta+n,\alpha+n})],\\
&\qquad\text{for } n\geq\alpha\geq\beta\geq 1,\\
P_{\alpha\beta}&=-i2^{-1/2}[(E_{\alpha\beta}-E_{\beta\alpha})+(E_{\alpha+n,\beta+n}-E_{\beta+n,\alpha+n})],\\
q_{\alpha\beta}&=[(E_{\alpha,\beta+n}-E_{\beta,\alpha+n})-(E_{\alpha+n,\beta}-E_{\beta+n,\alpha})],\\
p_{\alpha\beta}&=-i[(E_{\alpha,\beta+n}-E_{\beta,\alpha+n})+(E_{\alpha+n,\beta}-E_{\beta+n,\alpha})],\\
&\qquad\text{for } n\geq\alpha>\beta\geq 1,
\end{aligned} \tag{21}$$

where $E_{\alpha\beta}$ denotes the $2n\times 2n$ matrix whose only nonzero entry is one at the intersection of row α with column β.

For the orbit of quasiparticle vacua, the isotropy subalgebra equals

$$h_R=\mathrm{span}\{Q_{hh'},P_{hh'},Q_{pp'},P_{pp'},q_{ph},p_{ph}\}, \tag{22}$$

where h, h' range over the hole states, the first A vectors with unit occupancy, and p, p' run over the particle states, the last $n-A$ vectors with zero occupancy. Thus, the complexification of h_R is just the span of $a_h^\dagger a_{h'}$, $a_p^\dagger a_{p'}$, a_pa_h, and $a_p^\dagger a_h^\dagger$. One may show that h_R is isomorphic to the Lie algebra $u(n)$ of the unitary group $U(n)$. In particular, important subalgebras of h_R are also unitary algebras,

$$u(A) = \mathrm{span}\{Q_{hh'}, P_{hh'}\}$$
$$u(n-A) = \mathrm{span}\{Q_{pp'}, P_{pp'}\}. \quad (23)$$

The isotropy subgroup is given by exponentiation of the algebra, $H_R = \exp(ih_R) \simeq U(n)$. Moreover, the dimension of the quasiparticle vacuum orbit is $\dim O_R = \dim O(2n) - \dim U(n) = n(2n-1) - n^2 = n(n-1)$.

Note also that the isotropy subalgebra which fixes the quasiparticle vacuum density R contains precisely the operators which fix the corresponding determinantal wave function itself. Hence, the vacuum quasiparticle densities are in one-to-one correspondence with the vacuum quasiparticle wave functions.

The tangent space h_R^1 at R is computed to be

$$h_R^1 = \mathrm{span}\{Q_{ph}, P_{ph}, q_{hh'}, p_{hh'}, q_{pp'}, p_{pp'}\}, \quad (24)$$

and its complexification is hence the span of $a_p^\dagger a_h$, $a_h a_{h'}$, $a_p a_{p'}$, and their Hermitian conjugates. The symplectic form at R is zero for each pair of tangent vectors in Eq. (24) with the exception of

$$\omega_R(Q_{ph}, P_{ph}) = -\omega_R(P_{ph}, Q_{ph}) = -1,$$
$$\omega_R(q_{hh'}, p_{hh'}) = -\omega_R(p_{hh'}, q_{hh'}) = +1, \quad h \neq h', \quad (25)$$
$$\omega_R(q_{pp'}, p_{pp'}) = -\omega_R(p_{pp'}, q_{pp'}) = -1, \quad p \neq p',$$

It follows that ω is nondegenerate at R.

The tangent space at gRg^{-1} is $gh_R^1 g^{-1}$, which is spanned by $\{Q_{ph}(g), P_{ph}(g), q_{hh'}(g), p_{hh'}(g), q_{pp'}(g), p_{pp'}(g)\}$, where $Q_{ph}(g) = gQ_{ph}g^{-1}$, etc. Since the orthogonal transformations are canonical, Eq. (20), the symplectic structure ω at gRg^{-1} assumes the same form with respect to the basis $Q_{ph}(g), P_{ph}(g), \ldots$ as it did at R with respect to the basis $Q_{ph}, P_{ph}, \ldots$, Eq. (25). Thus, ω is nondegenerate at every point on the orbit O_R.

In the case of the generic orbits, the isotropy subalgebra is given by the diagonal matrices in $o(2n)$, and its complexification is spanned by $\{a_\alpha^\dagger a_\alpha - \frac{1}{2},\ \alpha = 1, 2, \ldots, n\}$. The generic isotropy subgroup is $U(1)x \ldots xU(1)$ (n copies). Hence, the dimension of the generic orbits is $\dim O_R = 2n(n-1)$.

Observe that the isotropy algebra elements which fix a generic density R do not fix the corresponding nondeterminantal wave function Φ. Indeed, there is only one $O(2n)$ generator which fixes Φ, viz. $\sum_\alpha (a_\alpha^\dagger a_\alpha - \frac{1}{2})$. Therefore, the $O(2n)$ orbit of wave functions has dimension $n(2n-1)-1$, and the correspondence between the orbit of wave functions and the orbit of densities is many to one.

The tangent space h_R^1 at R is given by the matrices in $o(2n)$ which have every diagonal entry zero and thus equals

$$h_R^1 = \mathrm{span}\{Q_{\alpha\beta}, P_{\alpha\beta}, q_{\alpha\beta}, p_{\alpha\beta}, n \geq \alpha > \beta \geq 1\}. \quad (26)$$

The only pairs of tengent vectors for which the symplectic form is nonzero are

$$\omega_R(Q_{\alpha\beta}, P_{\alpha\beta}) = -\omega_R(P_{\alpha\beta}, Q_{\alpha\beta}) = \nu_\alpha - \nu_\beta,$$
$$\omega_R(q_{\alpha\beta}, p_{\alpha\beta}) = -\omega_R(p_{\alpha\beta}, q_{\alpha\beta}) = \nu_\alpha + \nu_\beta - 1. \quad (27)$$

Therefore, for the generic orbits, the form is nondegenerate.

Once again, the tangent space at gRg^{-1} is $gh_R^1 g^{-1}$; it is spanned by $\{Q_{\alpha\beta}(g), P_{\alpha\beta}(g), q_{\alpha\beta}(g), p_{\alpha\beta}(g), \alpha > \beta\}$. Moreover, the symplectic form takes the same nondegenerate representation at gRg^{-1} as at R, c.f. Eqs. (20) and (27).

III. QUASIPARTICLE DYNAMICS

Due to the symplectic structure on the co-adjoint orbits of quasiparticle densities, classical Hamiltonian dynamics is defined on them. The crucial approximation is that the time development of an initial density R is a curve constrained to the orbit O_R. But then the tangent vectors to such curves at any point are elements of the orthogonal Lie algebra. The set of all tangent vectors to these constrained curves form the generalized Hartree-Fock-Bogoliubov Hamiltonian.

One would like to inherit the generalized HFB Hamiltonian from the microscopic interaction, as is achieved in conventional HFB. First, however, the usual HFB Hamiltonian is derived for the orbit of quasiparticle vacua.

Quasiparticle vacua

Let Φ be a Slater determinant and $a_\alpha^\dagger, a_\alpha$ be the single-particle fermion operators with respect to which $\rho = \mathrm{diag}(1, 1, \ldots, 1, 0, \ldots, 0)$ and R is diagonal, Eqs. (6), (7), and (14). At the point $\hat{g}\Phi$, the exact Hamiltonian $\hat{H}$ defines a curve $\gamma(t) = \exp(-i\hat{H}t)\hat{g}\Phi$ of states through the point $\hat{g}\Phi$, which are not in general quasiparticle vacua. Thus, $\hat{H}$ is not tangent to the orbit of quasiparticle vacuum wave functions. On the other hand, the Hartree-Fock-Bogoliubov Hamiltonian $\hat{H}_{\mathrm{HFB}}(\hat{g}\Phi)$ is a vector at $\hat{g}\Phi$ which is, by definition, tangent to the orbit surface and, therefore, an element of the orthogonal Lie algebra. Equivalently, because of the one-to-one identification with the orbit of quasiparticle vacuum densities, the HFB Hamiltonian is a vector field $H_{\mathrm{HFB}}(gRg^{-1})$ on the idempotent density surface.

The energy function on O_R is the expectation of the exact Hamiltonian,

$$H(gRg^{-1}) \equiv \langle \hat{g}\Phi \,|\, \hat{H}\hat{g}\Phi \rangle, \quad (28)$$

and its derivative in the direction of $Z \in o(2n)$ is

$$d\mathcal{H}(Z)=\frac{d}{dt}\langle\exp(-it\hat{Z})\hat{g}\Phi\,|\,\hat{H}\exp(-it\hat{Z})\hat{g}\Phi\rangle\,|_{t=0},$$
$$=-i\langle\hat{g}\Phi\,|\,[\hat{H},\hat{Z}]\hat{g}\Phi\rangle. \tag{29}$$

The HFB Hamiltonian is the element of $o(2n)$ satisfying

$$\omega_{gRg^{-1}}(H_{\mathrm{HFB}}(gRg^{-1}),Z)=d\mathcal{H}(Z), \tag{30}$$

for every tangent vector Z in $o(2n)$, c.f. Ref. 10. Since the symplectic form is nondegenerate, there is a unique solution for the HFB Hamiltonian,

$$H_{\mathrm{HFB}}(gRg^{-1})_{\alpha\beta}=(r_\alpha-r_\beta)^{-1}\langle\hat{g}\Phi|\,[\hat{H},d^\dagger_\beta(g)d_\alpha(g)]\,\hat{g}\Phi\rangle, \tag{31}$$

where r_α denotes the diagonal entries of R, Eq. (14), or

$$H_{\mathrm{HFB}}(gRg^{-1})_{\alpha\beta}=(r_\alpha-r_\beta)^{-1}\langle\Phi|\,[\hat{g}^{-1}\hat{H}\hat{g},d^\dagger_\beta d_\alpha]\,\Phi\rangle \tag{32}$$

Writing $\hat{H}$ explicitly as

$$\hat{H}=\sum_{\alpha\beta}^{n}T_{\alpha\beta}a^\dagger_\alpha a_\beta+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}^{n}V_{\alpha\beta\gamma\delta}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$
$$=\sum_{\alpha\beta}^{2n}T(g)_{\alpha\beta}d^\dagger_\alpha(g)d_\beta(g)$$
$$+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}^{2n}V(g)_{\alpha\beta\gamma\delta}d^\dagger_\alpha(g)d^\dagger_\beta(g)d_\delta(g)d_\gamma(g), \tag{33}$$

where

$$T(g)_{\alpha\beta}=\sum_{\alpha'\beta'}^{n}g^{-1}_{\alpha\alpha'}T_{\alpha'\beta'}g_{\beta'\beta},$$
$$V(g)_{\alpha\beta\gamma\delta}=\sum_{\alpha'\beta'\gamma'\delta'}^{n}g^{-1}_{\alpha\alpha'}g^{-1}_{\beta\beta'}V_{\alpha'\beta'\gamma'\delta'}g_{\gamma'\gamma}g_{\delta'\delta}. \tag{34}$$

Then, $\hat{g}^{-1}\hat{H}\hat{g}$ is given by Eq. (33) upon the substitutions $d^\dagger_\alpha(g)\to d^\dagger_\alpha$ and $d_\alpha(g)\to d_\alpha$. After evaluating the commutator and expectation in Eq. (32), the standard HFB Hamiltonian is obtained,

$$H_{\mathrm{HFB}}(gRg^{-1})=g^{-1}\begin{pmatrix}H_{\mathrm{HF}} & \Delta\\ -\Delta^* & -H^t_{\mathrm{HF}}\end{pmatrix}g, \tag{35}$$

where

$$(H_{\mathrm{HF}})_{\alpha\beta}=T_{\alpha\beta}+\sum_{\mu\nu}^{n}V_{\alpha\mu\beta\nu}\rho_{\nu\mu},$$
$$\Delta_{\alpha\beta}=\tfrac{1}{2}\sum_{\mu\nu}^{n}V_{\alpha\beta\mu\nu}t_{\mu\nu}. \tag{36}$$

Note that the HF Hamiltonian and the pair potential both depend upon g, since ρ and t do:

$$\begin{pmatrix}\rho & t\\ t^\dagger & 1-\rho^t\end{pmatrix}=g\begin{pmatrix}\nu_1 & & & & & & \\ & \ddots & & & & & \\ & & \nu_n & & & & \\ & & & 1-\nu_1 & & & \\ & & & & \ddots & & \\ & & & & & 1-\nu_n & \end{pmatrix}g^{-1}, \tag{37}$$

where the occupancies ν_α are zero or one for the quasiparticle vacuum orbit.

Generic orbits

In order to derive the HFB Hamiltonian on the generic orbits, the same construction is applied that proved successful for the orbit of quasiparticle vacua. All that is required is the specification of the energy function on the generic orbit O_R; the HFB Hamiltonian then follows immediately by reasoning similar to that in Eqs. (29)–(35).

However, the energy function cannot be just the expectation of the exact Hamiltonian, c.f. Eq. (28). The difficulty is that, in contrast to the quasiparticle vacuum orbit, the correspondence between the orbit of states and the generic orbit of densities, $\hat{g}\Phi\to gRg^{-1}$, is not one to one. Indeed, every state of the form $\hat{g}\hat{h}\Phi$ as h ranges over H_R is mapped onto the same density gRg^{-1}. But, the energy expectation $\langle\hat{g}\hat{h}\Phi\,|\,\hat{H}\hat{g}\hat{h}\Phi\rangle$ varies, in general, with $h\in H_R$. Thus, the exact Hamiltonian cannot be immediately transferred from the orbit of states to the generic density orbits.

The simplest resolution of this ambiguity is to average the energy over the states. Therefore, the energy function on the generic orbit O_R is defined by

$$\mathcal{H}(gRg^{-1})\equiv\int_{H_R}d\mu(h)\langle\hat{g}\hat{h}\Phi|\,\hat{H}\hat{g}\hat{h}\Phi\rangle. \tag{38}$$

The invariant measure on $H_R=U(1)x\cdots xU(1)$ is

$$d\mu(h)=\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\cdots\frac{d\theta_n}{2\pi}. \tag{39}$$

Following the construction in Eqs. (29)–(32), the generic HFB Hamiltonian is given by

$$H_{\mathrm{HFB}}(gRg^{-1})_{\alpha\beta}=(r_\alpha-r_\beta)^{-1}$$
$$\times\int_{H_R}d\mu(h)\langle\hat{h}\Phi|\,[\hat{g}^{-1}\hat{H}\hat{g},d^\dagger_\beta d_\alpha]\,\hat{h}\Phi\rangle. \tag{40}$$

For the one-body part of $\hat{H}$, the integrand is independent of $h \in H_R$ and averaging produces no effect. There is no ambiguity in transferring an operator in the $o(2n)$ algebra from the orbit of states to the orbit of densities. On the other hand, the two-body part requires averaging. Here one needs to use repeatedly the equation

$$\int_{H_R} d\mu\,(h)\langle \hat{h}\Phi | a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \hat{h}\Phi\rangle = (\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\delta})\langle \Phi | a_\alpha^\dagger a_\alpha a_\beta^\dagger a_\beta \Phi\rangle . \tag{41}$$

The final result for the HFB Hamiltonian on the generic orbits is

$$H_{\mathrm{HFB}}(gRg^{-1}) = g^{-1}\begin{pmatrix} H_{\mathrm{HF}} & \Delta \\ -\Delta^* & -H_{\mathrm{HF}}^t \end{pmatrix} g + \begin{pmatrix} X & Y \\ -Y^* & -X^t \end{pmatrix}, \tag{42}$$

$$X_{\alpha\beta} = \sum_{\delta=1}^{n} [V(g)_{\alpha\delta\beta\delta} - V(g)_{\alpha d\beta d} - V(g)_{b\delta a\delta} + V(g)_{bdad} + V(g)_{b\alpha a\delta} + V(g)_{d\delta a\beta}](R^\delta_{\alpha\beta} - \nu_\delta), \tag{43a}$$

$$Y_{\alpha\beta} = \sum_{\delta=1}^{n} [V(g)_{\alpha\delta b\delta} - V(g)_{\alpha dbd} - V(g)_{\beta\delta a\delta} + V(g)_{\beta dad} + V(g)_{\beta\alpha d\delta} + V(g)_{d\delta ab}](G^\delta_{\alpha\beta} - \nu_\delta), \tag{43b}$$

$$R^\delta_{\alpha\beta} = (\nu_\alpha - \nu_\beta)^{-1}\langle \Phi | (a_\alpha^\dagger a_\alpha - a_\beta^\dagger a_\beta) a_\delta^\dagger a_\delta \Phi\rangle , \tag{44a}$$

$$G^\delta_{\alpha\beta} = (\nu_\alpha + \nu_\beta - 1)^{-1}\langle \Phi | (a_\alpha^\dagger a_\alpha + a_\beta^\dagger a_\beta - 1) a_\delta^\dagger a_\delta \Phi\rangle , \tag{44b}$$

and $a = \alpha + n$, $b = \beta + n$, and $d = \delta + n$.

HFB solutions

An HFB solution is a critical point of the energy function on the orbit O_R[9]. Hence, at a solution, $d\mathcal{H}(Z) = 0$ for every direction Z in $o(2n)$, Eq. (29). But, from the nondegeneracy of ω, this requires the HFB Hamiltonian to have zero matrix elements corresponding to every tangent direction, Eqs. (24) and (26). In particular, for the generic orbits, the HFB matrix must be diagonal at a stationary state. Even for the quasiparticle vacuum orbit, although not required by the theory, it is customary to completely diagonalize the HFB matrix for the sake of convenience.

When constraints are imposed, then the Lagrange multiplier method is used to locate the critical points. For example, consider the constraint on particle number A. A constrained HFB solution is a critical point of the energy function restricted to the submanifold of O_R given by

$$\{gRg^{-1} \in O_R | \mathcal{N}(gRg^{-1}) = A\}, \tag{45}$$

where

$$\mathcal{N}(gRg^{-1}) = \mathrm{tr}(gRg^{-1}N), \qquad N = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \tag{46a}$$

defines the expectation of the number operator in $O(2n)$,

$$\mathcal{N}(gRg^{-1}) = \left\langle \hat{g}\Phi \left| \sum_{\alpha=1}^{n} a_\alpha^\dagger a_\alpha \hat{g}\Phi \right\rangle \right. . \tag{46b}$$

There exists a real number λ, the Lagrange multiplier, such that this constrained solution is a critical point in O_R to $\mathcal{H} - \lambda N$. Hence, $d\mathcal{H}(Z) - \lambda dN(Z) = 0$ for *every* tangent vector Z in $o(2n)$. But, from the nondegeneracy of ω, this means that the matrix

$$H_{\mathrm{HFB}}(gRg^{-1}) - \lambda gNg^{-1} \tag{47}$$

is diagonal at the critical point.

IV. DISCUSSION

A generalization of HFB has been achieved which is not restricted to quasiparticle vacua. The generalization begins with an arbitrary many-body state Φ and chooses a single-particle basis so that the HFB density matrix R is diagonal. Then, the coefficients $R^\delta_{\alpha\beta}$ and $G^\delta_{\alpha\beta}$ are calculated, Eq. (44). The generalized HFB Hamiltonian, a vector field tangent to the orbit O_R, is given by Eq. (42). A generalized HFB solution with the usual constraint on particle number is defined by a quasiparticle transformation g in $O(2n)$ and a Lagrange multiplier λ satisfying Eq. (45) for which the HFB matrix is diagonal, Eq. (47).

In the case of the quasiparticle vacuum orbit generated by a Slater determinant Φ, this construction reduces to the usual HFB theory. However, when $R^2 \neq R$, a new class of theories are obtained by this construction. The numerical solution for the HFB stationary states is achieved most easily with the Newton method.[11]

The average energy on the orbit surface is only one of the possible energy functions which determine a generalized HFB Hamiltonian, Eq. (38). For example, another sensible choice for the energy on O_R is given by

$$\mathcal{H}(gRg^{-1}) = \min_{h \in H_R} \langle \hat{g}\hat{h}\Phi | \hat{H}\hat{g}\hat{h}\Phi\rangle . \tag{48}$$

Which energy function is best is determined by the functional dependence of the energy expectation on h in H_R. If that expectation is only mildly dependent on h, then both energy functions are similar. The average energy is preferred then since it is easier to compute. However, if the energy expectation is a strongly dependent function of h in H_R with a sharp, deep minimum, then Eq. (48) is more suitable for zero temperature nuclei. At nonzero temperatures, yet a third energy function is presented by weighting the integrand of Eq. (38) with the Boltzmann factor.

It would be interesting to investigate the BCS

limit of this generalization. Note that the ideas used here also permit a generalization of the $SO(2n+1)$ model.[12]

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APPENDIX

Several results of a mathematical nature are collected into this Appendix. The isomorphism between the orthogonal Lie algebra $o(2n)$ and the algebra of bilinear products of fermion operators is demonstrated by explicit construction of the invariant inner product. See Refs. 6 and 7 for an alternate basis dependent proof. The $o(2n)$ algebra is then embedded in $u(2n)$ and expressed in terms of the conventional HFB formalism.

Isomorphism

Consider the real Lie algebra of skew-adjoint bilinear products of fermion operators,

$$\mathrm{bl}(n)=\mathrm{span}_R\{(\hat{C}_{\alpha\beta}-\hat{C}_{\beta\alpha}), i(\hat{C}_{\alpha\beta}+\hat{C}_{\beta\alpha}), (\hat{A}_{\alpha\beta}-\hat{B}_{\beta\alpha}), i(\hat{A}_{\alpha\beta}+\hat{B}_{\beta\alpha})\}, \tag{A1}$$

where

$$\begin{aligned}\hat{C}_{\alpha\beta}&=a_\alpha^\dagger a_\beta-\tfrac{1}{2}\delta_{\alpha\beta},\\ \hat{A}_{\alpha\beta}&=a_\alpha^\dagger a_\beta^\dagger,\\ \hat{B}_{\alpha\beta}&=a_\alpha a_\beta,\end{aligned} \tag{A2}$$

and $a_\alpha^\dagger$, a_α are the fermion creation and annihilation operators for the single-particle state α. It shall be proven that $\mathrm{bl}(n)$ is isomorphic to $o(2n)$, the real Lie algebra of the group of orthogonal transformations on a $2n$-dimensional real vector space V_{2n}.

Let V_{2n} denote the real span of the self-adjoint fermion operators,

$$\begin{aligned}e_\alpha&=2^{-1/2}(a_\alpha+a_\alpha^\dagger),\\ e_{\alpha+n}&=i2^{-1/2}(a_\alpha-a_\alpha^\dagger),\\ V_{2n}&=\left\{\zeta=\sum_{\alpha=1}^{n}(\zeta_\alpha e_\alpha+\zeta_{\alpha+n}e_{\alpha+n}),\ \zeta_j\in R\right\}.\end{aligned} \tag{A3}$$

Choose any normalized wave function Φ and define an inner product on V_{2n} by

$$\langle\zeta,\zeta'\rangle\equiv\langle\Phi\,|\,\{\zeta,\zeta'\}\Phi\rangle,\quad \zeta,\zeta'\in V_{2n}. \tag{A4}$$

Since the anticommutator is a multiple of the identity, the inner product is independent of the choice of Φ. With respect to the basis, $e_1, e_2, \ldots, e_{2n}$, the inner product defines the identity matrix and, hence, is nondegenerate.

The group given by exponentiation of the $\mathrm{bl}(n)$ algebra acts on V_{2n} by

$$\begin{aligned}&V_{2n}\to V_{2n},\\ &\zeta\to\exp(\hat{Z})\zeta\exp(-\hat{Z}),\ \hat{Z}\in\mathrm{bl}(n).\end{aligned} \tag{A5}$$

This transform of ζ is an element of V_{2n} because $[\zeta,\hat{Z}]\in V_{2n}$ and

$$\exp(\hat{Z})\zeta\exp(-\hat{Z})=\zeta+[\hat{Z},\zeta]+\frac{1}{2!}[\hat{Z},[\hat{Z},\zeta]]+\cdots. \tag{A6}$$

But, this transformation leaves invariant the inner product since

$$\begin{aligned}&\{\exp(\hat{Z})\zeta\exp(-\hat{Z}),\ \exp(\hat{Z})\zeta'\exp(-\hat{Z})\}\\ &\quad=\exp(\hat{Z})\{\zeta,\zeta'\}\exp(-\hat{Z})\\ &\quad=\{\zeta,\zeta'\}.\end{aligned} \tag{A7}$$

Therefore, it has been proven that the transformation (A5) is an orthogonal transformation of V_{2n}.

At the Lie algebra level, $\mathrm{bl}(n)$ infinitesimally preserves the inner product,

$$\langle[\hat{Z},\zeta],\zeta'\rangle+\langle\zeta,[\hat{Z},\zeta']\rangle=0, \tag{A8}$$

and $\mathrm{bl}(n)$ is isomorphic to the Lie algebra of the orthogonal group.

It is interesting to note that a similar argument shows that the bilinear products of boson operators is isomorphic to the symplectic Lie algebra $sp(n,R)$ (Ref. 13).

The isomorphism of $\mathrm{bl}(n)$ with $o(2n)$ immediately determines a representation of $\mathrm{bl}(n)$ by $2n\times 2n$ skew-symmetric matrices,

$$\hat{C}_{\alpha\beta}\to\tfrac{1}{2}\begin{pmatrix}(E_{\alpha\beta}-E_{\beta\alpha}) & -i(E_{\alpha\beta}+E_{\beta\alpha})\\ i(E_{\alpha\beta}+E_{\beta\alpha}) & (E_{\alpha\beta}-E_{\beta\alpha})\end{pmatrix}, \tag{A9}$$

$$\hat{A}_{\alpha\beta}\to\tfrac{1}{2}\begin{pmatrix}(E_{\alpha\beta}-E_{\beta\alpha}) & i(E_{\alpha\beta}-E_{\beta\alpha})\\ i(E_{\alpha\beta}-E_{\beta\alpha}) & -(E_{\alpha\beta}-E_{\beta\alpha})\end{pmatrix}, \tag{A10}$$

$$\hat{B}_{\alpha\beta}\to\tfrac{1}{2}\begin{pmatrix}(E_{\alpha\beta}-E_{\beta\alpha}) & -i(E_{\alpha\beta}-E_{\beta\alpha})\\ -i(E_{\alpha\beta}-E_{\beta\alpha}) & -(E_{\alpha\beta}-E_{\beta\alpha})\end{pmatrix}, \tag{A11}$$

where $E_{\alpha\beta}$ denotes the $n\times n$ matrix whose sole nonzero entry is one at the intersection of row α with column β.

Embedding of O(2n) in u(2n)

Conventional HFB is formulated with respect to the basis $\{a_\alpha^\dagger, a_\alpha\}$ of V_{2n}, instead of $\{e_\alpha, e_{\alpha+n}\}$. In order to express the $o(2n)$ algebra in the conven-

tional basis, it is necessary to make the unitary basis transformation given by the matrix

$$\Lambda=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\ 1 & i\end{pmatrix}. \tag{A12}$$

This transformation embeds $o(2n)$ as a subalgebra of $u(2n)$, the algebra of skew-adjoint $2n\times 2n$ matrices:

$$o(2n)\to u(2n),$$

$$\hat{C}_{\alpha\beta}\to\Lambda\tfrac{1}{2}\begin{pmatrix}(E_{\alpha\beta}-E_{\beta\alpha}) & -i(E_{\alpha\beta}+E_{\beta\alpha})\\ i(E_{\alpha\beta}+E_{\beta\alpha}) & (E_{\alpha\beta}-E_{\beta\alpha})\end{pmatrix}\Lambda^{\dagger}=\begin{pmatrix}E_{\alpha\beta} & 0\\ 0 & -E_{\beta\alpha}\end{pmatrix} \tag{A13}$$

and, similarly,

$$\hat{A}_{\alpha\beta}\to\begin{pmatrix}0 & E_{\alpha\beta}-E_{\beta\alpha}\\ 0 & 0\end{pmatrix}, \tag{A14}$$

$$\hat{B}_{\alpha\beta}\to\begin{pmatrix}0 & 0\\ E_{\alpha\beta}-E_{\beta\alpha} & 0\end{pmatrix}. \tag{A15}$$

Hence, a Hermitian operator $\hat{Z}$ in the complexified $bl(n)$ algebra,

$$\hat{Z}=\sum_{\alpha\beta}(X_{\alpha\beta}\hat{C}_{\alpha\beta}+\tfrac{1}{2}Y_{\alpha\beta}\hat{A}_{\alpha\beta}+\tfrac{1}{2}Y^{\dagger}_{\alpha\beta}\hat{B}_{\alpha\beta}), \tag{A16}$$

with X Hermitian and Y antisymmetric, is represented by the $2n\times 2n$ Hermitian matrix

$$Z=\begin{pmatrix}X & Y\\ Y^{\dagger} & -X^{t}\end{pmatrix}. \tag{A17}$$

An important inner automorphism of $o(2n)$ is given by

$$Z\to AZA^{-1}=-Z^{t}, \tag{A18}$$

where

$$A=\begin{pmatrix}0 & I\\ I & 0\end{pmatrix}.$$

Orthogonal group $O(2n)\subset U(2n)$

A quasiparticle transformation $g\in O(2n)\subset U(2n)$ must make $\Lambda^{\dagger}g\Lambda$ a real orthogonal matrix. Hence, we may write

$$g=\begin{pmatrix}u & v\\ v^{*} & u^{*}\end{pmatrix}, \tag{A19}$$

with $g^{\dagger}g=gg^{\dagger}=I$. Note also, since $\exp(iZ)$ is a group element, that $AgA^{-1}=g^{*}$.

In conventional HFB, the transformation to quasiparticles is completed by the transform

$$J=\begin{pmatrix}\rho & 1-\rho\\ 1-\rho & \rho\end{pmatrix},\quad \rho=\mathrm{diag}(1,1,\ldots,1,0,\ldots,0). \tag{A20}$$

Then, the generalized density is given by

$$R\to J\begin{pmatrix}\rho & 0\\ 0 & 1-\rho\end{pmatrix}J=\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}. \tag{A21}$$

A group transformation in this formalism is rewritten as,[8,9]

$$\begin{pmatrix}U & V\\ V^{*} & U^{*}\end{pmatrix}=Jg^{t}. \tag{A22}$$

This transform by J only simplifies notation for the quasiparticle vacuum orbit and offers no advantages for the general orbits. It has not been employed in this paper.

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